

HLWYM HEmails

From: Osvaldo Pensado
Sent: Wednesday, February 23, 2005 9:32 AM
To: vjain@cnwra.swri.edu; Roberto Pabalan
Cc: 'Darrell Dunn'; David Pickett; Jude McMurry
Subject: RE: ReferencepH--2

While I was at the OR office and checked the DOE model I learned that

- 1) in-package chemistry controls the rate of waste form degradation (not dissolution), colloidal stability, and solubility
- 2) the waste form needs to be in degraded form (e.g., schoepite) for radionuclides to be incorporated in solution
- 3) full degradation occurs in a few hundred years for SF (maybe few decades) and longer for HLW glass
- 4) if the temperature is above 100 centigrade, the waste form is assumed instantaneously degraded (measured degradation rates cannot be extrapolated beyond 100 C)
- 5) release into the geosphere is most likely to be in the form of a diffusive mechanism, because of the absence of seepage

Thus, I do not know what is the meaning of "conservative" with respect to in-package chemistry. The transport controlling factor is not clear to me. It is likely that in this convoluted model, the in-package chemistry may not be relevant at all.

-----Original Message-----

From: Vijay Jain [mailto:vjain@cnwra.swri.edu]
Sent: Wednesday, February 23, 2005 8:15 AM
To: rpabalan@cnwra.swri.edu; 'Osvaldo Pensado'
Cc: 'Darrell Dunn'; David Pickett; Jude McMurry
Subject: RE: ReferencepH

We need to look at our comments on TBD 7. I don't agree with the DOE abstraction and the range of pH values. I believe they are non-conservative.

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-----Original Message-----

From: Bobby Pabalan [mailto:rpabalan@cnwra.swri.edu]
Sent: Tuesday, February 22, 2005 4:49 PM
To: Osvaldo Pensado
Cc: Darrell Dunn; Vijay Jain
Subject: FW: ReferencepH

FYI.

-----Original Message-----

From: David Pickett [mailto:dpickett@cnwra.swri.edu]
Sent: Tuesday, February 22, 2005 4:35 PM
To: rpabalan@cnwra.swri.edu
Subject: RE: ReferencepH

Bobby,

Here's what DOE does for TSPA. In all cases, they use a uniform distribution between the min and max values for pH:

CSNF

For 0 to 600 years

min = 4.5

max = 7.0 to 8.1, depending on $f(\text{CO}_2)$. Model for the latter yields $f(\text{CO}_2)$ values that imply max pH of between 7.4 and 7.9.

For 600 to 20,000 years

min = 4.5

max = 7.0

Codisposal

For all times

min = 4.5

max = 7.0 for flux < 150 L/yr, 8.0 for flux > 150 L/yr

These seem reasonable to me. The lower limit (4.5) is based on 90 degree C simulations. If you want to only consider up to 50 degree C, the minimum could be 5.0. DOE models WP surface temperatures of >90 C up to 2000 years, and >50 C up to 13,000 years.

The maximum value of (usually) 7.0 is a function mainly of schoepite buffering. Higher pH is only modeled when water flux rates are high enough to reduce the effectiveness of the buffering. That explains the codisposal abstraction. Sitakanta tells me that flux > 150 L/yr is unlikely.

I conclude that, if we want to be consistent with the DOE in the absence of independent calculations, a uniform distribution between 4.5 and 7.0 would be reasonable. By the way, notes supporting this analysis are in notebook 172.

David

-----Original Message-----

From: Bobby Pabalan [mailto:rpabalan@cnwra.swri.edu]

Sent: Tuesday, February 22, 2005 4:12 PM

To: David Pickett

Subject: FW: ReferencepH

Any comments on this?

bobby

-----Original Message-----

From: Osvaldo Pensado [mailto:opensado@cnwra.swri.edu]

Sent: Tuesday, February 22, 2005 3:46 PM

To: Darrell Dunn; Vijay Jain; Roberto Pabalan

Subject: ReferencepH

There is a TPA parameter, ReferencepH, that is used only for spent fuel and glass dissolution rate determinations. That is to say, this pH value is an in-package value. I do not like using the normal distribution for two reasons: i) it has infinite tails, and ii) presumes that the additional information is available to defend the selection of normal distribution.

Instead, I propose using a uniform distribution. Otherwise, we could use a triangular distribution if you have a good guess of the most likely value (neutral pH maybe?).

Please comment ...

ReferencepH	pH of water	normal	3.6, 8.1	LB	EBSFAIL	477	Low upt OP pa de de ne dis
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